

LANSCE Los Alamos Neutron Science Center

LA-UR 13-23249

Name: **Prashant Jain**
Groups: **LANSCE-LC and MPA-CMMS**
Mentors: **Michael Fitzsimmons and Vivien Zapf**
Field of Study: **Chemistry**
Discipline: **Physical Chemistry**
Appointment: **Director's Postdoc Fellow**
Title: **Magnetoelectric Coupling in Multiferroic Metal-Organic-Frameworks (MOFs)**

Abstract

Multiferroics are rare materials with coexisting ferroelectric and ferromagnetic orders. Magnetoelectric multiferroics, wherein the two phenomena are coupled and can be manipulated by one another, are even rarer. Although there has been some success towards this end, most approaches involve controlling interactions at the interface between two different materials rather than switching of a single bulk phase. During the past decade there has been a resurgence of this field, which has primarily been driven by the exciting technological applications of magnetoelectric multiferroics. In this presentation, we will present our findings on single-phase multiferroic metal organic frameworks (MOFs). MOFs are crystalline materials composed of inorganic and organic building block with extended connectivity in at least one dimension. Most research in MOFs is focused on gas storage, separation, and catalysis; however, currently, we are interested in the condensed matter properties of these materials. In particular, we have shown that multiferroic behavior in MOFs is a new direction with advantages compared to the inorganic oxides. In addition, I will also present our latest results on magnetoelectric and magnetodielectric coupling in some of these novel materials.

LANSCE Los Alamos Neutron Science Center

LA-UR 13-23029

Name: **Rhiannon Meharchand**
Groups: **LANSCE-NS**
Mentors: **Fredrik Tovesson**
Field of Study: **Physics**
Discipline: **Nuclear Physics**
Appointment: **Director's Postdoc Fellow**
Title: **The NIFFTE Time Projection Chamber**

Abstract

Nuclear data such as cross sections, yields, angular distributions, energy spectra, and neutron multiplicity play a fundamental role in energy- and defense-related applications. Due in part to high development costs and testing restrictions, understanding of these applications has become increasingly dependent upon advanced simulation and modeling, where uncertainties in nuclear data propagate into uncertainties in calculated quantities and performance parameters. It is imperative therefore that nuclear data uncertainties are minimized and well-understood. To this end, the Neutron Induced Fission Fragment Tracking Experiment (NIFFTE) collaboration is developing a new experimental approach utilizing a Time Projection Chamber (TPC) to measure neutron-induced fission cross sections with unprecedented precision.

A novel detection system, the NIFFTE TPC combines existing technology – miniaturized and modified for use in nuclear physics – with state-of-the-art equipment. Frequent evaluation is required as hardware and software capabilities evolve. To evaluate progress, the TPC is tested in-beam at the Los Alamos Neutron Science Center (LANSCE) Weapons Neutron Research (WNR) facility. LANSCE-WNR, a spallation neutron source, provides a white neutron spectrum ranging from hundreds of keV to hundreds of MeV.

During the 2012 LANSCE run cycle, data were collected on several actinide samples, including U-238 and U-235. These data will be used to benchmark TPC performance and provide high-quality data to the community. An overview of the NIFFTE TPC project, the experiments performed at LANSCE-WNR, and preliminary performance results will be presented.

LANSCE Los Alamos Neutron Science Center

LA-UR 13-23072

Name: **Krista Meierbachtol**
Group: **LANSEC-NS**
Mentor: **Fredrik Tovesson**
Field of Study: **Physics**
Discipline: **Nuclear Physics**
Appointment: **Postdoc Research Associate**
Title: **SPIDER: A New Detector for Measuring Fission Yields**

Abstract

The study of fission fragment yields is important to both advance our understanding of the fission process and as a diagnostic tool for nuclear applications. A new detector, SPIDER (**S**Pectrometer for **I**on **D**etermination in fission **R**esearch) is being developed to measure fission yields as a function of incident neutron energy at LANSCE. The time-of-flight spectroscopy method being used by SPIDER, commonly referred to as the '2E-2v' method, measures the velocity and kinetic energy of the fission fragments in coincidence to identify their masses. Bragg spectroscopy will also be employed in combination with the energy measurement to determine the charge of each fragment. Prototype work on each detector component is on going and has indicated that 1 amu mass resolution can be achieved. The full scale SPIDER detector, an array, will increase detection efficiency and is currently being designed. The current status of SPIDER will be presented, including resolution capabilities and new results.

LANSCE Los Alamos Neutron Science Center

LA-UR 13-23030

Name: **Shea Mosby**
Group: **LANSCE-NS**
Mentor: **Aaron Couture**
Field of Study: **Physics**
Discipline: **Nuclear Physics**
Appointment: **Postdoc Research Associate**
Title: **High Energy Neutron Capture Cross Section of ^{239}Pu**

Abstract

High fidelity measurements of $^{239}\text{Pu}(n, g)$ are required for both nuclear energy campaigns and improved understanding of reaction diagnostics for defense programs. As part of the Advanced Reactor Concepts (ARC) program, new reactor designs are being considered for safe and cost-effective use in the United States and around the world. While traditional reactor designs have relied on light water reactors, the reactors planned for ARC will have a fast neutron spectrum, requiring improved nuclear data in the keV regime.

These measurements are particularly challenging on fissile isotopes as the fission gamma spectrum does not present unique features which can be used to discriminate fission gamma-rays from neutron capture. The Los Alamos Neutron Science Center (LANSCE) provides a high intensity neutron flux from thermal to several hundred keV. Coupled to this intense neutron source, the Detector for Advanced Neutron Capture Experiments (DANCE) provides a highly segmented 4π measurement of the gamma-ray energy and multiplicity distributions. Finally, a specially designed Parallel Plate Avalanche Counter (PPAC) detected coincidence fission fragments. Together, these instruments were used to provide a new high fidelity measurement of neutron capture on ^{239}Pu . Existing measurements extend up to 1 keV incident neutron energy, while measurements executed in the Spring of 2013 will push the measurement up to several hundred keV.

The simultaneous measurement of (n,g) and (n,f) events resulting from a single sample allowed the (n,g) cross section to be measured as a ratio to fission with reduced systematic uncertainty. Similar techniques applied to ^{235}U resulted in an uncertainty of 3% at 10 keV. Results from the current analysis on ^{239}Pu will be presented.

MPA Materials Physics and Applications Division

LA-UR 23170

Name: **Matthew DeVore**
Group: **MPA-CINT**
Mentor: **James Werner**
Field of Study: **Chemistry**
Discipline: **Physical Chemistry**
Appointment: **Postdoc Research Associate**
Title: **Simultaneous Fluorescence Imaging and Single-Molecule 3D Tracking in Live Cells**

Abstract

Although much is known about cellular endocytosis, questions remain concerning the step-by-step mechanisms and rates that govern the overall process. Activated receptors on a cell's plasma membrane often begin the process of endocytosis, the cellular uptake of target molecules by enveloping the targets in lipid vesicles formed from the plasma membrane. The vesicles are internalized by scission of the vesicle from the plasma membrane and active transport within the cell by motor proteins on the actin and microtubule network. The rates of vesicle budding and release from the membrane, the mechanism of vesicle handoffs between the actin and microtubule network, and the signaling competency of internalized receptors are still unknown for many receptors.

We are developing instrumentation to directly determine these properties for the IgE receptor FcεRI. The response of IgE-FcεRI to binding of a multi-valent antigen begins a cellular signaling cascade resulting in the release of histamine, part of the human allergic response. Previously, we have demonstrated three-dimensional tracking of individual fluorescently labeled IgE-FcεRI complexes diffusing on live cell membranes [1]. By adding the capability to fluorescently image specific cellular structures in wide field during a three-dimensional track of the IgE-FcεRI complex, we can investigate the signaling capability of the internalized receptor, directly see the transport of vesicles on the microtubule and actin networks, and determine the rates of vesicle budding and internalization. Here we present the incorporation of a Nipkow spinning disk into our tracking system to perform wide field fluorescence imaging and implementation of the change point analysis method [2] to determine diffusion coefficients of tracked molecules.

[1] Wells, Nathan P., et al. Nano Lett. 2010, 10, 4732-4737

[2] Montiel, D., et al. J. Phys. Chem. B 2006, 110, 19763-19770

MPA**Materials Physics and Applications Division**

LA-UR 13-23081

Name: **Aaron Keller**
Group: **MPA-CINT**
Mentors: **James Werner and Jennifer Hollingsworth**
Field of Study: **Chemistry**
Discipline: **Physical Chemistry**
Appointment: **Postdoc Research Associate**
Title: **3-Dimensional Tracking of Blinking-Suppressed Quantum Dots in Live Cells**

Abstract

Conventional fluorescence-based single molecule tracking methods are typically limited to tracking cellular processes in 2-dimensions at video frame rates (~ 30 frames/s), whereas many biophysical phenomena occur in 3-dimensional (3D) space on the submillisecond timescale over distances of several μm . For example, the endocytosis of Immunoglobulin E (IgE) during the down regulation of allergic response occurs over a distance of several μm and involves both diffusion at sub $\mu\text{m}^2/\text{s}$ rates and directed transport at nearly $1 \mu\text{m}/\text{s}$. Tracking such processes via fluorescence is further hindered by the unstable nature of many fluorophores which causes blinking (fluorescence intermittency) and/or photobleaching upon laser excitation. In order to observe spatio-temporal dynamics in 3D, we have previously developed a confocal 3D tracking microscope which maintains the fluorescent particle's position in the center of four spatially overlapping detection elements via feedback to a piezo stage. This 3D confocal based tracking can interrogate biophysical processes on the submillisecond timescale over distances of several μm . To suppress blinking and maintain fluorophore photostability, we implement so-called giant quantum dots (gQDs), containing a CdSe core with a number of CdS shells. The suppressed blinking in these gQDs allows the particles to be tracked in 3D for extended periods of time compared to the commercial QDs, which exhibit substantial blinking. Here we describe our methods for conjugating the gQDs to IgE and 3D tracking measurements that probe diffusion of the IgE-Fc ϵ RI complex on the surface of RBL mast cells as well as endocytosis after allergic stimulation. The extended tracking duration of the gQDs allows us to quantify heterogeneity in diffusion rates of individual IgE-Fc ϵ RI receptors. In the future, the use of blinking-suppressed gQDs for 3D tracking over extended periods of time and space is expected to be applicable to the study of many more biophysical processes.

MPA**Materials Physics and Applications Division**

LA-UR 13-23169

Name: **Wanyi Nie**
Groups: **MPA-CINT**
Mentors: **Aditya Mohite and Gautam Gupta**
Field of Study: **Physics**
Discipline: **Organic Optoelectronics**
Appointment: **Postdoc Research Associate**
Title: **Interface Modication for Organic Photovoltaic Devices**

Abstract

The organic photovoltaic devices have attracted great attention as the 3rd generation solar cell. However, the power conversion efficiency is still far behind the limit for scalable production. One of the major issues is the electron hole recombination at the interface, which is due to the high binding energy between electron-hole pair in the organic semiconductors. In our study, we show the by introduce a ultra-thin interface modification layer could reduce that recombination and result in a dramatic improvement in photocurrent. This material could both organic oligomer and inorganic material (i.e. LiF). We studied the charge transfer mechanism with such modification layer with impedance measurement.

MPA Materials Physics and Applications Division

LA-UR 13-22981

Name: **Douglas Shepherd**
Groups: **MPA-CINT and CCS-3**
Mentors: **James Werner and Brian Munsky**
Field of Study: **Physics**
Discipline: **Biophysics**
Appointment: **Postdoc Research Associate**
Title: **Counting Small RNA in Pathogenic Bacteria**

Abstract

Here, we present a modification to single-molecule fluorescence in situ hybridization that enables quantitative detection and analysis of small RNA (sRNA) expressed in bacteria. We show that short (~200 nucleotide) nucleic acid targets can be detected when the background of unbound singly dye-labeled DNA oligomers is reduced through hybridization with a set of complementary DNA oligomers labeled with a fluorescence quencher. By neutralizing the fluorescence from unbound probes, we were able to significantly reduce the number of false positives, allowing for accurate quantification of sRNA levels. Exploiting an automated, multi-color wide-field microscope and data analysis package, we analyzed the statistics of sRNA expression in thousands of individual bacteria. We found that only a small fraction of either *Yersinia pseudotuberculosis* or *Yersinia pestis* bacteria express the small RNAs YSR35 or YSP8, with the copy number typically between 1 and 10 transcripts. The numbers of these RNA are both increased (by a factor of 2.5× for YSR35 and 3.5× for YSP8) upon a temperature shift from 25 to 37 °C, suggesting they play a role in pathogenesis. The copy number distribution of sRNAs from bacteria-to-bacteria are well-fit with a bursting model of gene transcription. The ability to directly quantify expression level changes of sRNA in single cells as a function of external stimuli provides key information on the role of sRNA in cellular regulatory networks.

MPA Material Physics and Applications Division

LA-UR 13-20551

Name: **Navaneetha Subbaiyan**
Groups: **MPA-CINT and C-PCS**
Mentors: **Steve Doorn and Juan Duque**
Field of Study: **Chemistry**
Discipline: **Analytical Chemistry**
Appointment: **Postdoc Research Associate**
Title: **Photoinduced Electron Transfer Studies Using Supramolecular Porphyrin Based Model Systems**

Abstract

Photo induced electron transfer (PET) process results in generation of a charge-separated state between the excited donor and ground state acceptor moieties. Various factors that determine include exergonic free energy favoring charge separation, low solvent reorganization energy, desired distance and the orientation of the donor and the acceptor. Natural photosynthesis involves PET and results in harvesting the solar energy in useful form. Dye/pigment molecules are self-assembled in plants using supramolecular interactions to conduct PET events and generate starch from sunlight. Supramolecular chemistry - chemistry of non-covalent bonds includes different type of interactions such as ion-pairing, ion-dipole, dipole-dipole, hydrogen bonding, cation- π and Van der Waals forces. Mimicking natural photosynthesis to build solar devices has become important for generating either solar fuels or energy that could be stored for future use. Hence in this abstract, different supramolecular model system using porphyrins as donor and fullerenes as acceptor along with their design and construction are described. It is used to demonstrate the significance of solution and solid phase PET studies leading to the construction of supramolecular solar cells. The current finding could be applied to create interesting and interacting carbon materials based systems in search of next generation of efficient solar energy harvesting devices.

MPA Materials Physics and Applications Division

LA-UR 13-22980

Name: **Sibel Yalcin**
Group: **MPA-CINT**
Mentors: **Steve Doorn and Han Htoon**
Field of Study: **Materials Science**
Discipline: **Spectroscopy and Scanning Probe Microscopy**
Appointment: **Postdoc Research Associate**
Title: **Probing Charge Migration in Progressively Reduced Graphene Oxide using Electrostatic Force Microscopy**

Abstract

The discovery of graphene and tremendous attention it took in the last few years led to the discovery of graphene oxide (GO) for the large scale production of graphene. GO provides an ideal platform to manipulate and control its chemical structure, optoelectronic properties and ionic conductivity for a wide range of applications. Therefore, it is critical to understand the physical and electrical properties of GO that are highly dependent on the density and nature of functional groups. Here, using electrostatic force microscopy (EFM), we inject charge and directly probe the charge migration as the GO is progressively reduced (RGO). EFM results on GO flakes indicate that the injected charge is completely localized within the plane of GO. However, with the increasing degree of reduction, the injected charge rapidly delocalizes over a few microns until it ends up at the edge of the flakes. The results suggest that as we go from GO to RGO, there are more percolating pathways of sp² that are formed that act as conduits for charge migration. Our results are consistent with the observed photoluminescence quenching on GO flakes measured as a function of reduction from GO to RGO.

MPA Materials Physics and Applications Division

LA-UR 13-22982

Name: **Hisato Yamaguchi**
Group: **MPA-CINT**
Mentors: **Aditya Mohite and Steve Doorn**
Field of Study: **Materials Science**
Discipline: **Materials Synthesis and Optoelectronic Characterizations**
Appointment: **Director's Postdoc Fellow**
Title: **Correlated Photocurrent and Fluorescence Imaging from Individual Graphene Oxide Nanosheet**

Abstract

Graphene oxide (GO) is an attractive material as a precursor to grapheme. Structurally, GO is a grapheme sheet with oxygen-containing functional groups which are present in the form of carboxyl, hydroxyl and epoxy groups. GO is an electrical insulator due to disrupted conjugation of sp² bonds in the basal plane but can be controllably converted to a conductor via reduction. The fundamental limit of GO as an electronic material is that the functional groups cannot be removed completely, thus leaving a highly defective material with carrier mobilities that are orders of magnitude lower in comparison to exfoliated or even CVD grapheme. Despite its high degree of disorder, however, GO exhibits intriguing and unique properties that arise from “states” induced by the oxygen functional groups. One example is a tunable photoluminescence (PL), which can be tuned from blue to red by progressive chemical reduction. Our previous PL photocurrent microscopy (SPCM) and fluorescence with a diffraction limited spatial resolution, we report the optoelectronic properties of an individual GO flake as a function of controlled reduction. Progressive reduction of GO allows us to precisely control the lateral density of the sp² (graphitic) and sp³ (oxygen bearing) domains. This provides a strong handle in monitoring the evolution of photocurrent and understanding the role of oxygen bearing function groups that are involved in the PL. Furthermore, electric force microscopy (EFM) was used to investigate the charge migration within the single nanosheet and to map the local potentials as we transition from GO to reduced GO (RGO).

MPA Material Physics and Applications Division

LA-UR 13-23197

Name: **Jae Wook Kim**
Groups: **MPA-CMMS and LANSCE-LC**
Mentors: **Vivien Zapf and Michael Fitzsimmons**
Field of Study: **Physics**
Discipline: **Experiment in Condensed Matter and High Magnetic Field**
Appointment: **Postdoc Research Associate**
Title: **Coexistence of Ising and Heisenberg Moments in Multiferroic
Ca₃Co₂-xMnxO₆**

Abstract

We study the magnetic field-induced ordering of the multiferroic material Ca₃Co₂-xMnxO₆ (x~0.95) by measuring magnetization (M) and magnetostriction ($\Delta L/L$) up to magnetic fields of $\mu_0 H = 92$ T, which is beyond the saturation of the moments. We also investigate the electric polarization (P) up to 60 T and the magnetocaloric effect up to 50 T. On the controversial topic of the spin states of Co and Mn, we find evidence for S=3/2 Co²⁺ and Mn⁴⁺ spins with no magnetic field-induced spin-state crossovers. Our data also reveals a regime between 25 and 85 T in which the physical properties evolve smoothly, in contrast to the behavior below 25 T that is step-like and hysteretic. There is a universal linear slope in the background of magnetization curves for both H//ab and H//c. Thus we find that the Mn spins develop components in the ab-plane in applied magnetic fields that cant until saturation at 85 T, whereas Ising Co²⁺ spins saturate by 25 T. This implies that the Mn⁴⁺ spins are Heisenberg. On the low field region (<25 T), we find time-dependent features field dependent M, $\Delta L/L$, and P. This behavior is shown as two steps in magnetization and similar steps are found in other properties as well. Interestingly, it is only observed in certain sweep rates of magnetic field between 75 and 1500 T/s. This is similar to the sweep rate dependence of isostructural compound Ca₃Co₂O₆. Overall, our data show that this compound shows some of the hallmarks of ANNNI physics at low fields. However, at high fields it cannot be described by the classic ANNNI model, and models need to take into account the coexistence of Ising and Heisenberg spins.

MPA Material Physics and Applications Division

LA-UR 13-21238

Name: **Jianqiao Meng**
Group: **MPA-CMMS**
Mentor: **Tomasz Durakiewicz**
Field of Study: **Physics**
Discipline: **Condensed Matter Physics**
Appointment: **Director's Postdoc Fellow**
Title: **Photoemission Imaging of 3D Fermi Surface Pairing at the Hidden Order Transition in URu₂Si₂**

Abstract

We report angle-resolved photoemission spectroscopy (ARPES) experiments probing deep into the hidden order (H) state of URu₂Si₂, utilizing tunable photon energies with sufficient energy and momentum resolution to detect the near Fermi surface (FS) behavior. Our results reveal: 1) the full itinerancy of the 5f electrons; 2) the crucial three-dimensional (3D) k-space nature of the FS and its critical nesting vectors, in good comparison with density-function theory calculations; and 3) the existence of hot spot lines and pairing of states at the FS, leading to FS gapping in the HO phase.

MPA Materials Physics and Applications Division

LA-UR 13-23076

Name: **Brad Ramshaw**
Groups: **MPA-CMMS and NSEC**
Mentors: **Neil Harrsion and Albert Migliori**
Field of Study: **Physics**
Discipline: **Condensed Matter Physics**
Appointment: **Postdoc Research Associate**
Title: **Probing Fluctuations Above Superconductivity in PuCoGa5 with Resonant Ultrasound Spectroscopy**

Abstract

Plutonium metal is well known for its itinerant-localized crossover behaviour, possibly driven by valence fluctuations of its 5f electrons. Cerium 115 heavy Fermion systems exhibit a rich phase diagram with a range of correlated phenomena, including Kondo physics and superconductivity. The novel PuCoGa5 material combines the correlated physics of the 115s with the challenging and important problem of understanding the 5f electrons in plutonium. Using resonant ultrasound spectroscopy (RUS), we measure the elastic constants of PuCoGa5 to low temperatures, and observe a clear thermodynamic signature of superconductivity. In addition, we observe an anomalous fluctuation regime in a broad temperature range above T_c , and our symmetry analysis of these fluctuations in different elastic moduli is consistent with volume-changing valence fluctuations.

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MPA Materials Physics and Applications Division

LA-UR 13-23076

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Mentors: **Neil Harrsion and Albert Migliori**
Field of Study: **Physics**
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Abstract

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MPA**Materials Physics and Applications Division**

LA-UR 13-23068

Name: **William Rice**
Group: **MPA-CMMS**
Mentor: **Scott Crooker**
Field of Study: **Physics**
Discipline: **Condensed Matter Physics**
Appointment: **Postdoc Research Associate**
Title: **Optically Induced Magnetism in Reduced Strontium Titanate**

Abstract

When strontium titanate (SrTiO_3 or STO), a wide bandgap semiconductor that is a known quantum paraelectric, is paired with lanthanum aluminum oxide (LaAlO_3 or LAO), the 2D interface between the two becomes a high density electron gas ($\sim 10^{14} \text{ cm}^{-2}$), which is completely unexpected given that both STO and LAO are insulators. Researchers focusing on this interface have observed physically interesting, but often times conflicting, effects, such as strong electron correlations, metal-insulator transitions, coexistence of superconductivity and ferromagnetism, and electronic phase separation. The experimental picture is further complicated by evidence that oxygen vacancies in STO may play a part in some of these experimental observations, since every oxygen atom removed from STO adds two electrons. With a strong theoretical understanding of LAO/STO still lacking, there is strong incentive to shift focus to the individual components of this structure. Surprisingly, given the interest in LAO/STO, comparatively little research has been done on the magnetic and optical properties of STO itself.

Using magnetic circular dichroism (MCD) and SQUID magnetometry, we show the ability to create and control optically induced magnetism with sub-bandgap light in reduced STO (SrTiO_{3-d}) at low temperatures. When STO is reduced, we observe the appearance of two absorption peaks, one at 400 nm and a larger one at 430 nm, suggesting that sub-bandgap states are being created by the introduction of oxygen vacancies. Above measured carrier concentrations of 10^{12} cm^{-3} , we demonstrate that SrTiO_{3-d} can be magnetized by optically pumping at one of these absorption peaks with circularly polarized light. We show that this optically generated magnetism can be flipped when the optical pump is changed from right to left circular polarization. When the light is linearly polarized, no induced signal is observed. This polarization dependence implies that a net polarized spin population is created in SrTiO_{3-d} by changing the angular momentum of the pump photon. Furthermore, the magnetization can be flipped by changing the sub-bandgap photon pump wavelength from 400 nm to 425 nm. Interestingly, these optically induced effects are only seen below 20 K. To further investigate this temperature dependence, we measured the relaxation time dynamics of the induced signal as temperature was varied. As the sample temperature is decreased from 20 to 3 K, the relaxation time increases from seconds to tens of hours, indicating that we are pumping a metastable state. We show that the relaxation time temperature dependence follows an activated behavior with a 22 meV barrier.

To establish that oxygen vacancies are responsible for the long-lived optically induced magnetism, we reoxygenated a reduced STO sample. The addition of oxygen back into SrTiO_{3-d} completely quenched both the optical absorption features and the optically induced magnetization, confirming oxygen vacancies are responsible for both effects. In addition, other STO dopants, such as Nb and Fe, did not produce any of the interesting magneto-optical behaviors seen in SrTiO_{3-d} . This research shows that oxygen

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MPA Materials Physics and Applications Division

LA-UR 13-23068

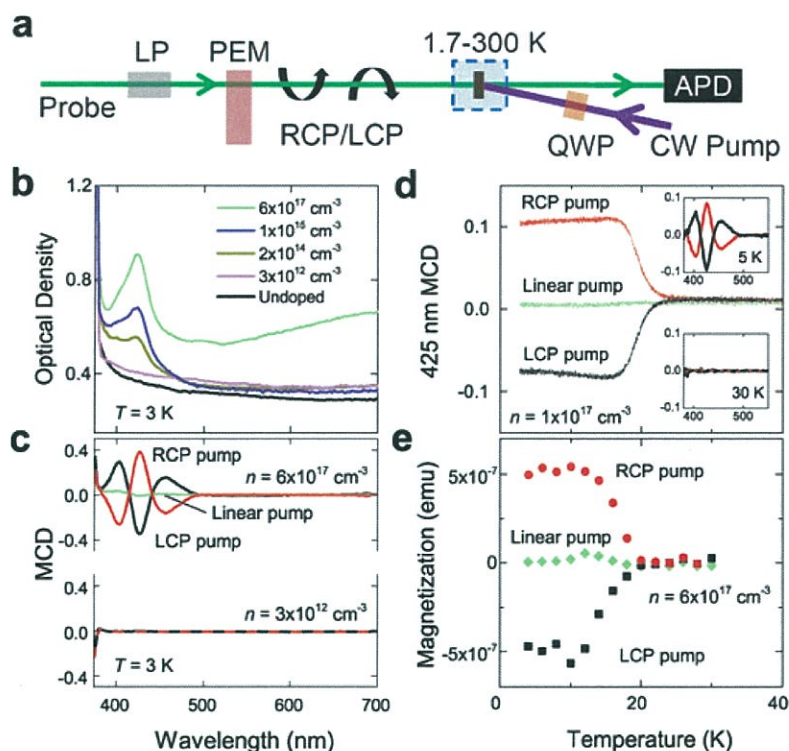
Name: **William Rice (*continued*)**
 Group: **MPA-CMMS**
 Mentor: **Scott Crooker**
 Field of Study: **Physics**
 Discipline: **Condensed Matter Physics**
 Appointment: **Postdoc Research Associate**
 Title: **Optically Induced Magnetism in Reduced Strontium Titanate**

Abstract

Continued from previous page

vacancies play a critical role in the magneto-optical behavior of STO and may lead to a deeper understanding of the physics involved in LAO/STO interfaces.

To establish that oxygen vacancies are responsible for the long-lived optically induced magnetism, we reoxygenated a reduced STO sample. The addition of oxygen back into SrTiO_{3-d} completely quenched both the optical absorption features and the optically induced magnetization, confirming oxygen vacancies are responsible for both effects. In addition, other STO dopants, such as Nb and Fe, did not produce any of the interesting magneto-optical behaviors seen in SrTiO_{3-d} . This research shows that oxygen vacancies play a critical role in the magneto-optical behavior of STO and may lead to a deeper understanding of the physics involved in LAO/STO interfaces.



MPA**Materials Physics & Applications Division**

LA-UR 13-23075

Name: **Arkady Shehter**
Groups: **MPA-CMMS and NSEC**
Mentors: **Jon Betts and Albert Migliori**
Field of Study: **Physics**
Discipline: **Condensed Matter Physics**
Appointment: **Postdoc Research Associate**
Title: **Bounding the Pseudogap in the High Temperature Superconducting Cuprates**

Abstract

Close to optimal doping, the copper oxide superconductors show ‘strange metal’ behaviour, suggestive of strong fluctuations associated with a quantum critical point. Such a critical point requires a line of classical phase transitions terminating at zero temperature near optimal doping inside the superconducting ‘dome’. The underdoped region of the temperature-doping phase diagram from which superconductivity emerges is referred to as the ‘pseudogap’ because evidence exists for partial gapping of the conduction electrons, but so far there is no compelling thermodynamic evidence as to whether the pseudogap is a distinct phase or a continuous evolution of physical properties on cooling. Here we report that the pseudogap in $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$ is a distinct phase, bounded by a line of phase transitions. The doping dependence of this line is such that it terminates at zero temperature inside the superconducting dome. From this we conclude that quantum criticality drives the strange metallic behaviour and therefore superconductivity in the cuprates.

MPA Materials Physics and Applications Division

LA-UR 13-22868

Name: **Brian Rekken**
Group: **MPA-MSID**
Mentor: **Benjamin Davis**
Field of Study: **Chemistry**
Discipline: **Inorganic Chemistry**
Appointment: **Postdoc Research Associate**
Abstract Title: **Fluid-Phase Hydrogen Storage using Amine-Borane Ionic Liquids**

Abstract

Efficient storage of H₂ may enable a new energy paradigm for a variety of applications, including vehicular, stationary, and portable technologies. Several modalities have been examined, including metal hydrides, absorbents, and chemical compounds. Of the latter class, the blend of ammonia-borane and ionic liquids emerged as a strong candidate for compact hydrogen storage technologies and is a promising alternative to petroleum for meeting our everyday energy needs. However, current iterations will solidify upon dehydrogenation to give an intractable solid, incapable of quick refueling. In light of this, we have developed a new class of N-substituted amine-boranes tethered to ionic liquid moieties. The compounds were prepared through a multi-step synthesis and characterized by standard techniques. Thermogravimetric decomposition (DSC, TGA) of said compounds revealed exothermic degradation similar to ammonia-borane. Several derivatives of the pure amine-boranes and mixtures with ammonia-borane were shown to co-oligomerize during hydrogen release to give liquid products and thereby demonstrate their viability as material to meet the Department of Energy's ultimate targets for transitioning to a hydrogen fuelled economy.

MPA**Materials Physics and Applications Division**

LA-UR 13-23742

Name: **Neil Tomson**
Groups: **MPA-MSID**
Mentors: **James Boncella**
Field of Study: **Chemistry**
Discipline: **Molecular Actinide**
Appointment: **Postdoc Research Associate**
Title: **Molecular U(IV) Mono(imido) Chemistry: New Starting Materials and Imido-group Reactivity**

Abstract

Compared to the high-valent bis(imido) complexes $U(NR)_2X_2L_n$, mono(imido) U(IV) species exhibit N-based reactivity consistent with greater polarization of the U–N multiple bond. Characterization of this interaction has been hampered, however, by the lack of suitable starting materials for investigating this chemistry in a step-wise fashion. Nearly all of the known U(IV) mono(imido) compounds contain cyclopentadienide or bulky-amido co-ligands, stretching the relevance of comparisons between these different species. Building on a recently developed methodology for generating mononuclear, mono(imido) U(IV) dihalides, we report the synthesis and characterization of products resulting from imido-group reactivity at several U(IV)-imido-containing compounds. In particular, treatment of the U-complexes with aryl, alkyl, and silyl isocyanates is shown to lead to various reaction products, which highlights the divergent reactivity available to uranium imido complexes that span differing oxidation states.

MST Materials Science and Technology Division

LA-UR 13-23125

Name: **Nikolaus Cordes**
Groups: **MST-7**
Mentors: **Brian M. Patterson**
Field of Study: **Materials Science**
Discipline: **X-ray Microscopy**
Appointment: **Postdoc Research Associate**
Title: **Characterization of Metal Doped Polymer Capsules using Confocal Micro X-ray Fluorescence Spectroscopy and X-ray Computed Tomography**

Abstract

Defect Induced Mix Experiment (DIME) spherical capsules, utilized as National Ignition Facility (NIF) targets, are composed of a 42 μm -thick polymer shell which has been doped with a 2 μm -thick inner layer of 1.5 at.% germanium and a 2 μm -thick outer layer of 1.5 at.% gallium. The metal-doped layers are separated by a 3 μm -thick polymer layer. The LANL DIME campaign requires that the characterization of these capsules must provide better accuracy than the fabrication tolerances.

This poster will describe the nondestructive characterization of DIME capsules using a variety of X-ray techniques including confocal micro x-ray fluorescence (MXRF) spectroscopy, Micro and Nano X-ray Computed Tomography (CT). While the qualitative characterization of the metal dopant regions of DIME capsules using confocal MXRF is relatively straightforward, the quantitative characterization of these regions is a non-trivial task. In order to quantify the germanium concentrations, thin germanium films of sequential thicknesses were fabricated and utilized to calibrate the confocal MXRF instrument. Sample-to-sample variations in metal concentrations were also investigated using statistical analysis of the confocal MXRF data. Micro and Nano X-ray CT of DIME capsules will also be presented. The non-destructive analysis of DIME capsules using CT allows for the imaging and quantification of polymer and metal-dopant region thicknesses, as well as imaging of induced defects on the capsule equatorial plane.

MST Materials Science & Technology Division

LA-UR 13-23058

Name: **Matthew N. Lee**
Groups: **MST-7**
Mentors: **Kimberly Obrey**
Field of Study: **Materials Science**
Discipline:
Appointment: **Postdoc Research Associate**
Title: **A New Class of Porous and Composite Materials Based on Colloidal Assembly at Fluid Interfaces**

Abstract

Colloidal particles can stabilize fluid interfaces in a manner similar to amphiphilic surfactants. A key difference however is that particles can become trapped at an interface with adsorption energies orders of magnitude greater than the thermal energy, kT , effectively “locking in” a non-equilibrium configuration of the fluid species. This phenomenon enables a robust bottom-up approach for synthesis of functional materials with well-defined microstructure using colloidal particles with tunable chemistry and geometry as building blocks. Familiar examples are particle-stabilized (Pickering) emulsions and foams, which are widely utilized in consumer products, oil recovery, foods, and pharmaceuticals. In this research, self-assembly of colloidal particles at fluid interfaces is used to direct the microstructure and functionality of a new class of porous and composite materials based on bicontinuous emulsions. Here, colloidal particles with specific wetting properties kinetically arrest spinodal decomposition of a partially-miscible liquid pair. The resultant non-equilibrium microstructure, known as a bicontinuous interfacially-jammed emulsion gel, or bijel, is then used as a general platform to synthesize a novel family of bicontinuous macroporous, hierarchically porous, and composite materials with tunable chemistry and morphology. The assembly of particles at the interface provides a means to percolate their properties in composite structures and generate hierarchical assemblies on widely separated length scales. This flexible, scalable, and inexpensive approach allows for the rational design of microstructured materials for diverse applications in catalysis, separations, tissue engineering, and renewable energy systems.

MST Materials Science & Technology

LA-UR 13-23192

Name: **Joshua White**
Group: **MST-7**
Mentor: **Andrew Nelson**
Field of Study: **Materials Science**
Discipline: **Ceramics and Nuclear Engineering**
Appointment: **Postdoc Research Associate**
Abstract Title: **Thermal Conductivity of Oxygen-Rich Uranium Dioxide**

Abstract

Oxidation of the fuel meat in light water reactors occurs when UO_2 at elevated temperatures is exposed to the water coolant. The thermal conductivity is dramatically decreased with increased oxygen content, but the fundamental mechanisms are largely unknown. Oxygen stoichiometries of UO_2 specimens ranging from 2.000 to 2.210 were prepared in situ within thermoanalytical equipment. Thermogravimetric analysis of UO_2 specimens under the hybrid gas environments provides insight into the oxidation kinetics of UO_2 to UO_{2+x} under varying partial pressures of oxygen. Thermal conductivities were analyzed according to Klemens-Callaway model. Analysis of the data sets allows for extraction of the fundamental phonon-phonon and phonon-defect scattering contributions for the materials investigated. This fundamental dataset provides a key contribution to ongoing efforts in the modeling and simulation communities in the areas of both light water reactor fuel performance and accident evolution.

MST-8 Materials Science & Technology

LA-UR 13-23303

Name: **Benjamin Morrow**
Group: **MST-8**
Mentors: **Ellen Cerreta and Carlos Tome**
Field of Study: **Materials Science**
Discipline: **Metallurgy and Characterization and Structure/Property Relationships**
Appointment: **Postdoc Research Associate**
Abstract Title: **TEM In-Situ Straining Experiments in Magnesium**

Abstract

Due to a limited number of available slip systems, both slip and twinning are important for deformation in magnesium. In order to fully understand this behavior, it is necessary to characterize the interactions between dislocations and twins, and the impact of these interactions on subsequent deformation. Additionally, these interactions may have implications towards detwinning, an important component to fatigue behavior. In-situ transmission electron microscopy (TEM) was used to directly observe the microstructure during deformation. Ex-situ (post-mortem) TEM was performed on samples compressed in an orientation favorable for {10-12} twinning to provide complementary information about the active processes. This characterization will provide a more complete understanding of the substructural evolution during deformation to help to guide and improve future efforts to model behavior in HCP metals.

MST**Materials Science and Technology**

LA-UR 13-23042

Name: **Shuai Shao**
Groups: **MST-8 and MPA-CINT**
Mentors: **Jian Wang, Carlos Tome, and Amit Misra**
Field of Study: **Materials Science**
Discipline: **Nanoscale Multilayered Composites (Modeling)**
Appointment: **Postdoc Research Associate**
Abstract Title: **The Structure, Evolution, and Radiation Damage Resistance of FCC (111) Semi-Coherent Interfaces**

Abstract

In nuclear reactors, the high dosage of alpha and neutron radiation bombard the atoms to displace up to hundreds of times which generates various types of defects such as vacancies, self-interstitials, He bubbles etc. Such defects severely damage structural materials over their service life, e.g. radiation hardening, swelling and He embrittlement. Thus, over the last few decades, there has been a renewed interest among the research community to search for new types of materials that can substantially withstand the damage caused by the radiation. The nanoscale metallic multilayers offer such ability as the point defects have low formation energy and high diffusivity at the interfaces. In this work, we bring one of such interfaces, the FCC (111) semi-coherent interface, into focus by performing atomistic simulations on the Cu-Ni platform. We studied the structure of the interface and the misfit dislocation network resides therein. An important dislocation nodal structure evolution, the nodal expansion, is found to occur when the interface is subject to shear loading or upon the addition of an interstitial atom. Such evolution significantly reduces the formation energies of the irradiation-induced point defects in the nodes, which potentially improves the radiation damage resistance of the interface.

NSEC National Security Education Center

LA-UR 13-23133

Name: **Steven Anton**
Group: **NSEC**
Mentor: **Chuck Farrar**
Field of Study: **Engineering**
Discipline: **Mechanical Engineering**
Appointment: **Postdoc Research Associate**
Abstract Title: **Multi-Source Energy Harvesting to Power Remote Sensing Systems**

Abstract

Approximately 50% of black carbon (BC) aerosols come from wildfires and are estimated to contribute up to ~ 0.6 W/m² warming of the atmosphere globally. Organic carbon (OC) from fires condenses and/or mixes with BC resulting in an overall lower forcing of 0.03 ± 0.12 Wm⁻² from biomass burning. However, this reduction depends strongly on the composition of the carbonaceous aerosols and on the mixing state of OC and BC. Detailed model treatments and laboratory measurements indicate that a BC core coated with a nonabsorbing OC layer enhances absorption with a positive climate forcing. However, the real-time identification of the coating on this internally mixed BC in the field has only recently become detectable with the analysis of lag times between the scattering and incandescence signals in measurements from the single particle soot photometer (SP2). Direct on-line measurements of BC are made with the SP2, which measures the mass of the particles by incandescence on an individual particle basis, from nearby and aged wildfires in addition to those produced in the laboratory. We investigate BC in concentrated wildfire plumes from the two largest wildfires in New Mexico's history with different ages and compare them to BC from indoor generation from single-source fuels, e.g. ponderosa pine, sampled during the Fire Lab At Missoula Experiments IV (FLAME-IV) at the US Forest Service Rocky Mountain Research Station's Fire Science Laboratory in Missoula, Montana in November of 2012. Plumes from the Las Conchas (LC) Fire, a wildfire that occurred in July-August of 2011 and burned ~ 157 K acres, were sampled in the near-field after only a few hours of aging. Older plumes from the Whitewater Baldy (WB) Fire (May-June, 2012) that burned ~ 300 K acres were sampled from further afield with an aging period of 7-9 hours. FLAME-IV includes real-time sampling from direct emissions, well-mixed samples, and aging studies.

P Physics Division

LA-UR 13-23203

Name: **Chaitanya Chandrana**
Group: **P-21**
Mentor: **Pulak Nath**
Field of Study: **Physics**
Discipline: **Nuclear Magnetic Resonance**
Appointment: **Postdoc Research Associate**
Abstract Title: **Towards Automated Fabrication of Halbach Rings for NMR Applications**

Abstract

We present a novel approach to automatically arrange multiple permanent magnets in a Halbach orientation for NMR/MRI applications. The Halbach array is a special arrangement of multiple magnets that superimpose magnetic fields from individual magnets to produce uniform magnetic field distribution. Using Finite Element Analysis, we have observed that a diametrically magnetized cylindrical magnet can produce a magnetic field distribution that mimics the polarization of an ideal Halbach ring. Therefore, we utilized a diametrically magnetized cylinder to simultaneously and automatically align multiple magnets into a Halbach assembly. This approach dramatically reduces the complexities associated with fabricating Halbach arrays. Prototypes were built using NdFeB magnets and NMR relaxometry was performed on water samples doped with CuSO₄.

P Physics Division

LA-UR 13-22996

Name: **Young Jin Kim**
Group: **P-21**
Mentors: **Andrei Matlashov and Michelle Espy**
Field of Study: **Physics**
Discipline: **Physics**
Appointment: **Postdoc Research Associate**
Abstract Title: **Development of a Pulsed ^{14}N Quadrupole Resonance Technique for the Solid Explosives Detection**

Abstract

At present, Nuclear Magnetic Resonance (NMR) has been shown to be useful in the detection of liquid explosives. However, although NMR is a powerful tool for liquid explosive detection, it is unsuitable to detect solid explosives due primarily to their short transverse relaxation times. Nuclear Quadrupole Resonance (NQR) is a promising alternative technique both because no magnetic field is required and because the transverse relaxation times are much longer. In NQR, a nucleus that contains a nuclear quadrupole moment couples to the internal electric field gradient from the surrounding electronic structure of the nucleus. This leads to the nuclear energy level splitting, without a holding field as in NMR, which varies with different nuclear species. This makes NQR an exceptional method in distinguishing different materials. Most solid explosives contain measurable concentrations of the quadrupolar nucleus ^{14}N that can be detected by NQR with a high degree of accuracy.

We have developed our first-ever fully homemade portable NQR probe designed to operate in ^{14}N NQR frequency ranges from 0.4 to 5 MHz. We have successfully observed the 4.64 MHz NQR signal from sodium nitrite. SNR was ~ 40 after 50 data sets average. The probe was also used to measure relaxation times (T_1 and T_2) of the sodium nitrite sample using standard pulse sequences. To improve the NQR signal detection, efforts are underway to use polarization enhancement techniques. For that, we will test ammonium nitrate because it is of significant interest, it has NQR modes at frequencies less than 500 kHz (thus is difficult to detect), and has both ^{14}N and ^1H nuclei. Results of the NQR measurements will be presented. After demonstrating polarization enhancement, we will combine an existing low field NMR/MRI system at LANL with the NQR system for simultaneous liquid and solid explosives detection.

P Physics Division

LA-UR 13-23667

Name: **Jennie Schei**
Groups: **P-21 and MPA-MSID**
Mentors: **John George and Andrew Dattelbaum**
Field of Study: **Physics**
Discipline: **Biophysics**
Appointment: **Director's Postdoc Fellow**
Abstract Title: **Implications of Microscopic Eye Movements for Retinal Encoding**

Abstract

Vision is one of the most important sensory systems humans use to explore the surrounding environment, and a large brain region is dedicated to processing visual information. As a visual stimulus enters the retina, pixel intensity information is not directly encoded. Rather, several preprocessing steps occur and then encoded signals are sent through the optic nerve to the visual cortex as a temporal sequence of transient responses called spikes. During fixed gaze, the eyes make microscopic eye movements that may aid in the perception of fine spatial detail. We hypothesize that microscopic eye movements temporally modulate the visual stimulus and encode spatial feature relationships through precisely timed, spatially coherent neurons. Furthermore, these eye movements may enhance detection and learning of visual features. We employed a model of the outer retina developed by van Hateren (expanded to 32x32 array of photoreceptors, with electrical coupling between horizontal cells), coupled to spiking models of the inner retina and primary visual cortex, implemented in our package Petavision. We introduced a noisy Gabor image stimulus and simulated microscopic eye movements in both one and two dimensions. Movement orthogonal to the grating orientation blurred structure and reduced contrast encoded by spike rate; however, a reconstruction using temporal covariance enhanced spatial detail. In contrast, movement parallel to the grating orientation enhanced periodic modulation and reduced high frequency noise encoded by spike rate. Random two-dimensional movement blurred the output representations of the gratings, but enhanced the representation encoded by correlations within the image. In electrophysiological studies, we simulated microscopic eye movements by jittering a visual stimulus on an isolated retina (tiger salamander) and recording spiking using a multi-electrode array. The retinal ganglion cell spiking rate increased and synchronized to the jitter frequency. Together, the modeling and electrophysiological studies suggest that microscopic eye movements may enhance feature representation of visual information by encoding of temporal correlations within populations of neurons.

P Physics Division

LA-UR 13-20171

Name: **Jacob Yoder**
Group: **P-21**
Mentors: **Michelle Espy and Andrei Matlashov**
Field of Study: **Physics**
Discipline: **Nuclear Magnetic Resonance**
Appointment: **Postdoc Research Associate**
Abstract Title: **Measuring Absolute Water Content of Trees in Vivo by Lowe Field NMR in an Uncontrolled Environment**

Abstract

The resilience of trees in drought conditions is one of the key factors to the long term survival of forests under changing climate conditions and therefore an important factor in estimating carbon storage for climate models. It is important to understand the movement and storage of water in trees in order to get at the mechanisms of hydraulic failure during a drought; current tools generally involve probes that penetrate the tree and therefore seriously alter the measurement. NMR is potentially the best technique available for measuring water content of trees or plants in vivo; it is completely nondestructive and the signal is directly proportional to water content when the signal from the wood is excluded. Most work to date has been done in temperature controlled environments, with the notable exception of the “Tree Hugger” permanent magnet based NMR/MRI system. We describe in this work a pre-polarized, un-cooled, electromagnet based system designed to measure water content of trees <35mm in diameter. We discuss in detail the many systematic effects due to variation in environmental temperature and how these effects can be corrected to measure absolute water content precisely. Preliminary results with a sapling apple tree and sticks are presented.

P Physics Division

LA-UR 13-23151

Name: **Leah Broussard**
Group: **P-25**
Mentor: **Mark Makela**
Field of Study: **Physics**
Discipline: **Neutron Physics**
Appointment: **Seaborg Postdoctoral Fellow**
Abstract Title: **Ultra-Cold Neutron Physics at the Los Alamos Neutron Science Center**

Abstract

The Ultra-Cold Neutron (UCN) program at the Los Alamos Neutron Science Center (LANSCE) facility at the Los Alamos National Laboratory uses one of the highest density sources of UCN in the world to perform high precision measurements of neutron decay observables. The UCNA collaboration has recently published a sub-percent measurement of the beta-asymmetry, $A_0 = -0.11952(110)$, and has completed a new data-taking cycle which implemented significant improvements to reduce all major systematic effects. The UCNB experiment is expected to perform a preliminary measurement of the neutrino-asymmetry B at the 0.1% level during the 2013 run cycle, and has shown the capability for very low-noise operation at full bias voltage and magnetic field. The UCNTau collaboration has recently performed a successful demonstration of the UCN storage trap, which a trap storage time of about 10 hours. Finally, a new program is now being developed which will use UCNs to characterize material sputtering due to fission in actinides such as plutonium. An overview of the UCN programs and latest results will be presented.

T Theoretical Division

LA-UR 13-22962

Name: **Ondrej Certik**
Group: **T-1**
Mentor: **Lee Collins**
Field of Study: **Physics**
Discipline: **High Energy Density Physics**
Appointment: **Postdoc Research Associate**
Abstract Title: **Real Space Finite Element Methods in Orbital-Free Molecular Dynamics**

Abstract

The area of warm, dense matter (WDM) has received considerable attention recently due its identification with an assortment of environments as diverse as the interiors of exoplanets, the atmospheres of stars, inertial confinement fusion capsules, and the plasma from laser interactions with materials from clusters to nanostructures.

The WDM regime presents a particularly difficult challenge given that quantum mechanical effects play a crucial role in the accurate representation of this complex medium under extreme conditions. This regime severely taxes current orbital-based Kohn-Sham (KS) density function theory (DFT) solvers. The high temperatures require large numbers of states and consequently, the diagonalization of huge matrices, leading to a very computationally expensive problem. In response to this limitation, orbital-free density functional methods, based only on a three-dimensional density, have received renewed attention.

The KS methods generally employ plane-waves as a basis as does the current orbital-free molecular dynamics code at LANL and must rely on Fast Fourier Transform (FFT) techniques for evaluation of the functional components. The FFT algorithm unfortunately does not scale well on parallel platforms as demonstrated in diverse applications. As such, the plane-wave DFT codes do not allow the efficient treatment of very large numbers of atoms over extended times, a condition essential to addressing future WDM problems. In order to accelerate such calculations, a better algorithm is needed for the Poisson solver whose implementation has in practice a better scaling behavior than FFT.

We show preliminary results using real space finite element methods. The finite element discrete variable representation, also known as the spectral element (SE) method, has exponential convergence, but unlike plane waves the basis functions are strictly local, thus are well suited for parallel solvers. Convergence graphs and other comparisons will be shown for model systems.

T Theoretical Division

LA-UR 13-22903

Name: **Jeffery Leiding**
Group: **T-1**
Mentor: **Joshua Coe**
Field of Study: **Chemistry**
Discipline: **Theoretical Chemistry**
Appointment: **Postdoc Research Associate**
Abstract Title: **An Efficient Method for Performing Ab Initio Monte Carlo Simulation**

Abstract

Atomistic Monte Carlo (MC) simulation is an important tool for calculating equilibrium properties of materials, particularly when sampling events (such as chemical reaction) that may be rare on time scales accessible to molecular dynamics (MD). MC sampling based on classical potentials has been performed extensively, but prior calibration of such potentials to data imbues them with a strongly a posteriori character relative to ab initio (AI) ones, which are often predictive. MC sampling of AI potentials has, however, heretofore been virtually nonexistent. This is due to MC samples of any sort being strongly correlated, such that many more energy evaluations are required than are statistically meaningful; if the cost of each evaluation is relatively high (as in the case of AI), the method is simply impractical. The efficiency of ab initio Monte Carlo (AIMC) is enhanced significantly through use a nested scheme: many-particle steps based on a classical reference potential are used to generate trial states for AI evaluation, and the form of the acceptance probability is adjusted accordingly. This statistically decorrelates configurations at which the AI potential must be evaluated, thereby sharply reducing variance in ensemble averages for a given number of samples. Previously Coe, et. al, found that the thermodynamic state (P, T) of the reference system could be varied so as to maximize the acceptance rate of nested steps by up to 3x, but at the expense of an additional simulation performed prior to production runs (needed to determine the optimal state of the reference system).

This work will demonstrate an on-the-fly reference system optimization that dramatically enhances AIMC efficiency in as few as 10 (unoptimized) MC steps. This circumvents the need to perform the extra simulation mentioned above, and accelerates variance reduction to the point AIMC efficiency becoming competitive with that of ab initio molecular dynamics. The method's performance will be illustrated using the Argon Hugoniot.

T Theoretical Division

LA-UR 13-23035

Name: **Hao Li**
Group: **T-1**
Mentor: **Sergei Tretiak**
Field of Study: **Chemistry**
Discipline: **Quantum and Computational Chemistry**
Appointment: **Postdoc Research Associate**
Abstract Title: **Appraisal of Orthogonalization Techniques of Atomic Wave Functions within the Exciton Scattering (ES) Theory**

Abstract

The exciton scattering (ES) approach is a multiscale technique developed for efficient calculations of spectroscopic observables in large low-dimensional conjugated molecular systems as an extension of commonly used quantum-chemical methods. Within the ES approach, electronic excitations in the quasi-one-dimensional molecular structure are attributed to standing waves that represent quantum quasi-particles (excitons) reside on the graph, whose edges and nodes stand for the molecular linear segments and vertices, respectively. Usually large conjugated molecules only consist of a limited number of molecular building blocks. Therefore, the electronic properties of the entire conjugated structure can be expressed in terms of the excitation data of elementary building blocks, which can be extracted from traditional quantum-chemical computations performed on molecules of interest of moderate size. This idea involves accurate estimates of electronic and excitonic properties for any molecular component.

Considering of the nonorthogonality of the atomic orbitals (AOs) used in ab initio quantum-chemical methods, followed by non-Hermitian terms in the Hamiltonian, which prevent accurate evaluation of physical quantities, a variety of orthonormalization techniques have been developed and became standard tools in common quantum-chemical packages. In our study, we studied several AO representations, including original AO, standard Löwdin orthogonalized AO, and natural atomic orbital (NAO) basis sets, to evaluate their quantitative performance for the ES approach. The comparison indicates that local excitation (transition charge and dipole moment) of arbitrary molecular component can be accurately estimated only under the NAO representation. Therefore, applying the ES approach, combined with the NAO analysis to optical spectra of branched conjugated oligomers, we accurately predict absorption spectra compared to the counterparts of the reference quantum-chemistry. This testifies applicability of a variety of quantum-chemical techniques, where the NAO population analysis can be conducted, for the ES theory.

T Theoretical Division

LA-UR 13-20551

Name: **Gopinath Subramanian**
Group: **T-1**
Mentors: **Art Voter and Danny Perez**
Field of Study: **Materials Science**
Discipline: **Computational Materials Science**
Appointment: **Postdoc Research Associate**
Abstract Title: **Informing Irradiation Creep and Growth Models Using an Object kMC that Couples Elasticity with Diffusion**

Abstract

This poster outlines an object kinetic Monte Carlo framework that is capable of accurately computing defect absorption rates by sinks – a key parameter in irradiation damage models. The results show that the strain field surrounding a sink enhances the absorption rate of point defects by a significant amount, and the enhancement is a strong function of the state variables. The results demonstrate the importance of a hitherto neglected phenomenon: strain-induced absorption rate enhancement, and highlight the perils of using averaged model parameters.

T Theoretical Division

LA-UR 13-22947

Name: **Fan Guo**
Group: **T-2 and XCP-6**
Mentors: **Hui Li and Bill Daughton**
Field of Study: **Astronomy**
Discipline: **Astrophysical Plasma Processes**
Appointment: **Postdoc Research Associate**
Abstract Title: **Particle Acceleration during Magnetic Reconnection in Pair Plasmas**

Abstract

Magnetic reconnection is a fundamental plasma process where magnetic field lines change topology and magnetic energy rapidly converts into kinetic energies of plasmas. Strong signatures of particle energization associated with magnetic reconnection have been observed, however the mechanism of acceleration remains poorly understood. Recently, gamma-ray flares at energies greater than 100 MeV from Crab pulsar have been observed by Fermi observatory, indicating an efficient particle acceleration driven by relativistic magnetic reconnection. PAMELA, Fermi and AMS space observatories detected an increasing positron/electron fraction with energies from ~ 10 GeV - ~ 100 GeV, possibly from nearby pulsars. It has been speculated that particle acceleration associated with magnetic reconnection in pair (electron-positron) plasmas may help explain these observations.

We utilize a 2-D particle-in-cell code that includes the full range of plasma physics to model particle acceleration during magnetic reconnection in pair plasmas. The acceleration processes are examined using the newly developed particle-tracking module. The simulations start from a current sheet on the skin-depth scale. The current sheet rapidly breaks at multiple locations (X-points) and forms magnetic islands (O-points). We identify the acceleration patterns and distinguish the contribution by X-points and O-points. We also examine the influences by guide field, inflow density, size of the simulation domain, etc. We find the non-ideal electric field parallel to the magnetic field play an important role when there exists a strong guide field.

T Theoretical Division

LA-UR 13-22938

Name: **Enrico Camporeale**
Group: **T-5**
Mentors: **Gian Luca Delzanno and Xianzhu Tang**
Field of Study: **Physics**
Discipline: **Plasma Physics**
Appointment: **Postdoc Research Associate**
Abstract Title: **Lower Hybrid to Whistler Mode Conversion on a Density Striation**

Abstract

When a wave packet composed of short wavelength lower hybrid modes traveling in an homogeneous plasma region encounters a density inhomogeneity, it can resonantly excite long wavelength whistler waves via a linear mechanism known as mode conversion. We study the linear mode conversion using a scalar-field formalism (in the limit of cold plasma linear theory) which we solve numerically [1]. We show that the linear mode conversion can effectively transfer a large amount of energy from the short to the long wavelength modes, and we study how the efficiency scales for different width and amplitude of the density striation. We present a general criterion for the width of the striation that, if fulfilled, maximizes the conversion efficiency. Such a criterion could provide an interpretation of recent laboratory experiments carried out on the Large Plasma Device at UCLA.

[1] E. Camporeale, G.L. Delzanno, P. Colestock, "Lower hybrid to whistler mode conversion on a density striation" (2012) J. Geophys. Res., 117, A10315.

T Theoretical Division

LA-UR 13-21384

Name: **Guangye Chen**
 Group: **T-5**
 Mentor: **Luis Chacon**
 Field of Study: **Physics**
 Discipline: **Computational Plasma Physics**
 Appointment: **Postdoc Research Associate**
 Abstract Title: **Fully Implicit, Energy- and Charge-conserving Particle-in-cell Algorithms for Kinetic Simulation of Plasmas**

Abstract

Particle-in-cell (PIC) simulation techniques have been wildly successful in the first-principles simulation of plasma dynamics. However, the fundamental algorithmic underpinnings of classical PIC algorithms have not changed in decades. The classical PIC method employs an explicit approach (leap-frog) to advance the Vlasov-Poisson/Maxwell system using particles coupled to a grid. Explicit PIC is subject to both temporal stability constraints (limiting the time step) and spatial stability constraints (requiring a minimum mesh cell size), which makes it unsuitable for long-term, system-scale kinetic simulations, even with modern super-computers.

Implicit PIC algorithms can potentially eliminate both spatial and temporal stability constraints, thus becoming orders of magnitude more efficient than explicit ones. This motivated much exploration of implicit PIC algorithms in the literature since the 1980's. However, the lack of efficient nonlinear solvers for a very large system of field-particle equations required approximations that resulted in intolerable accumulation of numerical errors in long-term system-scale simulations.

We will present a fully implicit, nonlinear one-dimensional PIC algorithm using a Jacobian-Free-Newton-Krylov method on a one-dimensional electrostatic model [1], targeting both accuracy and efficiency for multi-scale plasma kinetic simulations. The formulation conserves local charge and total energy exactly. Momentum is not exactly conserved, but errors are kept small by an adaptive particle sub-stepping orbit integrator. We have extended the formulation to mapped meshes, opening the possibility of accurate spatially adaptive PIC simulations [2]. The algorithm can be effectively accelerated with fluid models [3,4], and is ideally suited for GPU computing [5]. The superior accuracy and efficiency properties of the scheme will be demonstrated with challenging numerical examples. We will also discuss the extension of the approach to electromagnetic PIC in the non-relativistic regime via a Darwin model, which avoids noise issues associated with numerical Cherenkov radiation [6] while remaining exactly energy and charge conserving.

[1] G. Chen, L. Chacón, and D.C. Barnes, J. Comput. Phys., 230 (18), 7018 (2011) [2] L. Chacón, G. Chen, D. C. Barnes, J. Comput. Phys., 233, 1-9 (2013) [3] W. Taitano, D. Knoll, L. Chacón, G. Chen, SISC, submitted (2013) [4] G. Chen, L. Chacón, in preparation. [5] G. Chen, L. Chacón, D. C. Barnes, J. Comput. Phys., 231, 5374-5388 (2012) [6] S. Markidis and G. Lapenta, J. Comput. Phys., 230 (18), 7037 (2011)

T Theoretical Division

LA-UR 13-20796

Name: **Nathan Lemons**
Groups: **T-5 and T-CNLS**
Mentor: **Aric Hagberg**
Field of Study: **Mathematics and Computer Science**
Discipline: **Discrete Mathematics**
Appointment: **Postdoc Research Associate**
Abstract Title: **Phase Transition and Connectivity in Random Intersection Graphs**

Abstract

The well-studied Erdős-Rényi graph, $G(n,p)$, is a basic model for random networks that is amenable to structural analysis. However, $G(n,p)$ is not suited as a model for real-world networks; perhaps the most common criticism is that sparse realizations of $G(n,p)$ do not exhibit clustering. Thus $G(n,p)$ is not a good model for most social networks which are usually sparse and have nontrivial clustering. A simple natural model for networks which derive their structure from bipartite graphs (i.e. most social networks) is the random intersection graph. Random intersection graphs were first introduced by Karonski, Scheinerman and Singer-Cohen and have recently attracted much attention. This interest is due to the fact that random intersection graphs incorporate the bipartite structure found in many social networks. In particular they can exhibit nontrivial clustering while remaining sparse.

Issues of connectivity including the size of the largest components in random networks are fundamental. Here we determine exactly when the random intersection graph has a unique largest component. In particular, it is shown that there is a sharp phase transition. We also locate the threshold of connectivity for random intersection graphs.

WX Weapons Experiments Division

LA-UR 13-22837

Name: **Erik Moro**
Groups: **WX-4 and WX-3**
Mentors: **Matthew Briggs and Larry Hull**
Field of Study: **Engineering**
Discipline: **Optical Diagnostics**
Appointment: **Director's Fellow**
Abstract Title: **Extracting Transverse Motion from Speckle Dynamics in Photon Doppler Velocimetry**

Abstract

Photon Doppler velocimetry (PDV) is gaining increasing popularity as a test diagnostic at Los Alamos National Laboratory, where it is routinely used to measure velocities of explosively driven surfaces. Elsewhere, PDV's accuracy and robustness make it suitable for use in a wide range of test applications with velocities ranging from a few to several thousand meters per second. That being said, all optical velocimetry to date (PDV included) has been limited to measuring one spatial dimension per probe, and in the case of PDV, a probe measures a surface's velocity projected along its measurement beam's axis. A separate phenomenon, laser speckle, has been related to transverse speeds of less than 1 m/s (perpendicular to the beam's axis) in certain optical arrangements. Laser speckle manifests itself in PDV data as low-frequency, random amplitude fluctuations, and it has historically been viewed as a hindrance to velocity extraction. However, if speckle dynamics may be accurately related to transverse speed, it potentially enables an unmodified PDV system to simultaneously measure axial velocity (standard analysis approach) and transverse speed (speckle analysis) at each deployed probe.

In this presentation, we relate a surface's transverse speed to PDV laser speckle dynamics in three quantifiable ways - (1) the coherence time calculated from the data's autocorrelation properties, (2) the variance of the time-derivative of the data, and (3) the data's low-frequency content. We demonstrate that all three signal features have utility in calculating transverse speed, and we compare them to one another in terms of accuracy, uncertainty effects, and robustness in relating speckle dynamics to surface motion.

WX Weapons Experiments Division

LA-UR 13-22925

Name: **Joshua Coleman**
Group: **WX-5**
Mentors: **Carl Ekdahl and Dave Moir**
Field of Study: **Physics**
Discipline: **Accelerator and Plasma Physics**
Appointment: **Postdoc Research Associate**
Abstract Title: **Designing the Next Generation of Multi-Pulsed Intense Relativistic Electron Beams**

Abstract

The next generation of intense relativistic electron beams (IREB) will require a stable, multi-pulsed, well diagnosed beam. Current challenges with thermionic cathodes present the need for advanced cold cathode technologies, that can either be extracted with a single 2-us pulse or individually addressable multiple pulses through the injector. There are four components currently being addressed in order to achieve these goals: develop high brightness cold cathode technologies with minimal gap closure velocity, quantify the gap closure physics of relativistic electron beams with hollow anodes, develop non-invasive beam diagnostics, and increase performance characteristics of the current state-of-the-art IREB facility, DARHT. The experimental configurations are presented, which include a cold cathode test stand, DARHT Axis-1, the non-invasive diagnostics currently being developed and deployed, and a quantitative set of experimental results.

WX Weapons Experiments Division

LA-UR 13-20919

Name: **Eric Anderson**
Group: **WX-9**
Mentor: **Scott Jackson**
Field of Study: **Physics**
Discipline: **Shock and Detonation Physics**
Appointment: **Postdoc Research Associate**
Abstract Title: **Transverse Initiation of an Insensitive Explosive in a Layered Slab Geometry**

Abstract

Experiments are presented that explore the shock initiating layer dynamics in an insensitive high explosive. Tests were conducted with a PBX 9502 slab bonded on one side to a PBX 9501 slab. For each test, a planar detonation in the PBX 9501 was generated to drive a shock into the PBX 9502. The thickness of the PBX 9501 layer was varied to control the strength and duration of the transmitted shock. Phase velocities at the explosive outer surfaces, wave-front breakout shapes, and post-shock particle velocity histories associated with the detonating and initiating zones in the two explosives are reported and discussed.

WX Weapons Experiments Division

LA-UR 13-22998

Name: **Patrick Bowden**
Group: **WX-9**
Mentor : **Dana Dattelbaum**
Field of Study: **Physics**
Discipline: **Shock and Detonation Physics**
Appointment: **Postdoc Research Associate**
Abstract Title: **High Pressure-temperature Phase Behavior of 2, 4, 6 -Trinitrotoluene (TNT)**

Abstract

2,4,6-Trinitrotoluene (TNT) is an important energetic material due to its widespread use, and ability to be melt-cast, which stems from its low melting point, and chemical stability in the molten phase. Numerous studies have investigated the unreacted equation of state, shock initiation and detonation behavior of TNT. However, there are relatively few measurements on the structure-property relationships under static high pressure conditions. High pressure-temperature (P-T) Diamond Anvil Cell (DAC) studies with in-situ experimental probes such as vibrational spectroscopy and x-ray diffraction (XRD) provide critical thermodynamic data that are useful for modeling P-V-T behavior. At ambient conditions, TNT crystallizes in a monoclinic lattice (space group P2₁/a), and our previous x-ray diffraction (XRD) measurements at room temperature suggested a phase transition to orthorhombic (space group Pca2₁) at ~20 GPa. In this study, detailed Raman (60-4000 cm⁻¹) and infrared (40-4000 cm⁻¹) vibrational spectroscopy measurements and XRD data were collected using synchrotron radiation sources to investigate phase stability and previously reported phase transitions. Infrared and Raman spectra were obtained up to 21 GPa and 500 °C. Structural information was obtained using angle-dispersive x-ray diffraction across an extensive range of P-T conditions along isothermal and isobaric pathways up to 30 GPa and 500 °C. The ambient-pressure monoclinic polymorph has a rich vibrational spectrum with 45 modes in IR and 39 modes in Raman observed, of the 57 predicted normal modes. The pressure dependency of the vibrational modes revealed some unusual features, with deformation modes [δ (C-H), δ (CH₃), ρ (CH₃), and others] exhibiting minimal shifts with pressure, and splitting of several modes observed from 1-12 GPa. While our spectroscopy measurements indicate spectral changes at ~2 GPa, careful XRD measurements (hydrostatic, He medium and non-hydrostatic) reveal that the monoclinic phase is likely stable up to 20 GPa. Using all the available data, we have established the first comprehensive high P-T phase diagram of TNT, including the melting line as a function of pressure.

WX Weapons Experiments Division

LA-UR 13-22915

Name: **Kathryn Brown**
Group: **WX-9**
Mentor: **Dave Moore**
Field of Study: **Physics**
Discipline: **Shock Dynamics**
Appointment: **Agnew National Security Postdoc Fellow**
Abstract Title: **Transient Absorption and Hugoniot Equations of State of Shocked Nitromethane**

Abstract

We use transient absorption spectroscopy and ultrafast dynamic ellipsometry (UDE) to characterize reactions occurring in shocked nitromethane and nitromethane sensitized with diethylenetriamine (DETA). Sustained (~ 300 ps) shocks up to ~ 20 GPa were generated from an amplified Ti:sapphire laser. Nitromethane is an insensitive explosive liquid, and it is well known that the addition of an amine, such as DETA, increases its sensitivity to detonation. Though not chemical-specific, transient absorption and deviations from the universal liquid Hugoniot can indicate that chemical reactions are occurring and enhance the understanding of the reaction mechanisms. The information obtained from these experiments can be applied to more specific characterization methods such as vibrational spectroscopy.

WX Weapons Experiments Division

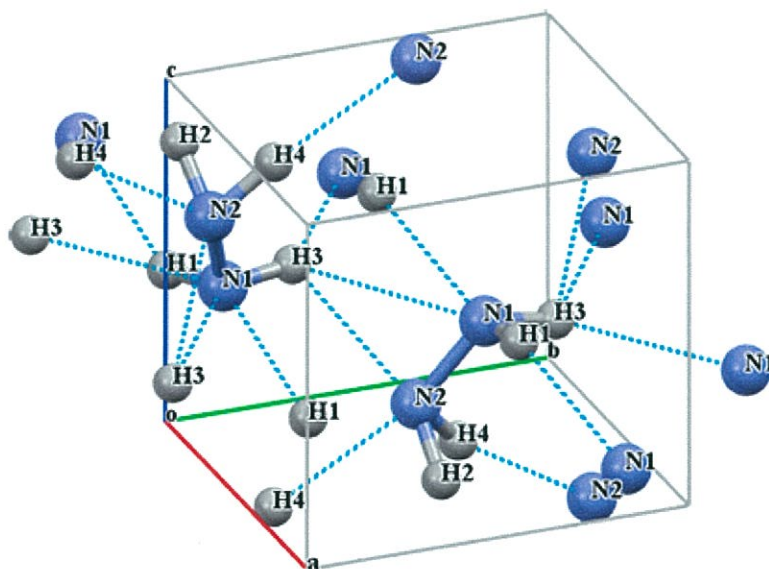
LA-UR 13-22967

Name: **Raja Chellappa**
 Group: **WX-9**
 Mentor: **Dana Dattelbaum**
 Field of Study: **Materials Science**
 Discipline: **Chemistry of Materials Science**
 Appointment: **Postdoc Research Associate**
 Abstract Title: **Energetic “Hydronitrogen” Solids: Insights from Behavior of Hydrogen Bonding (H-H...N) in Hydrazine (H₂N-NH₂) under Compression**

Abstract

Hydrazine (H₂N-NH₂) is a high-energy density molecule widely used in liquid propellant formulations and been implicated in planetary physics as well. High pressure/temperature (P/T) behavior of hydrazine is of interest to explore the role of compression in N-H...N hydrogen bond symmetrization and formation of 3-D networked polymeric extended “hydronitrogen” energetic solids. Several simple molecules with strong hydrogen bonding exhibit symmetrization (HCO₂H, H₂O) and form extended solids with potential for energetic applications. Here, we report the first comprehensive study of hydrazine to 20 GPa at ambient temperature, using *in situ* vibrational spectroscopy and synchrotron x-ray diffraction (XRD) to elucidate structural changes driven by compression and reorganization of N-H...N hydrogen bonding networks.

Liquid hydrazine solidifies at 0.3 GPa into a crystalline phase with a remarkable correspondence to its *low*-T monoclinic structure. For the first time, we have determined the structure of the high pressure phase of hydrazine. With increasing pressure, Raman & Infrared spectra reveal a directional strengthening of the hydrogen bonding in the 5-7 GPa range, that persists up to 20 GPa. While, no evidence for extended amorphous solids was observed to 20 GPa, this study provides a basis for investigating the role of a second component (similar to H₂-H₂O clathrate hydrates) in stabilizing the 3-D hydrogen bonding network in hydrazine at moderate pressures (<1 GPa).



WX Weapons Experiments Division

LA-UR 13-25296

Name: **Carlos Chiquete**
Group: **WX-9**
Mentor: **Mark Short**
Field of Study: **Physics**
Discipline: **Shock and Detonation Physics**
Appointment: **Postdoc Research Associate**
Abstract Title: **Non-linear and Linear Stability of Pulsating Overdriven Detonation with a Chain-branching Kinetics Model**

Abstract

The non-linear and linear dynamics of gaseous overdriven one-dimensional detonations with a two-step chain-branching kinetic mechanism are investigated. Stable detonations are obtained when the (state insensitive) main heat release layer is longer than the initial induction layer. Linear analyses reveal a destabilizing effect (with respect to the limiting Chapman-Jouguet case) for small overdrive. The corresponding nonlinear dynamics of the pulsating detonation are studied.

WX**Weapons Experiments Division**

LA-UR 13-22551

Name: **John Yeager**
Group: **WX-9**
Mentor: **Daniel Hooks**
Field of Study: **Materials Science**
Discipline: **Composites and Explosives**
Appointment: **Agnew National Security Postdoc Fellow**
Abstract Title: **Mesoscale Characterization of Plastic-Bonded Explosives Across Time and Length Scales**

Abstract

The performance, safety, and thermo-mechanical response of heterogeneous materials such as plastic-bonded explosives (PBXs) is inherently linked to microstructural phenomena. These microstructure-level details drive initiation, safety, and structural behaviors that have been historically categorized as “stochastic,” for lack of a better understanding of the local mechanisms. A mesoscale interpretation of the microstructure and its contribution to PBX properties is necessary to inform PBX damage and mechanical behavior models, to understand and predict failure of current explosives, and to design better explosives for future use. This research investigates the microstructural contributions to quasi-static and dynamic PBX behavior, with focus on the crystal-binder interface. The interface between the explosive crystals and the polymer binder is determined by formulation parameters and influences crack behavior and composite integrity. Several PBX formulations are studied to illustrate the effectiveness of the characterization methodology. Engineered PBX 9501 composites were studied with neutron reflectometry, showing that the nano-structure at the crystal-binder interface was altered when a plasticizing agent was included in the formulation. The plasticized interface resulted in worse adhesion between the binder and the crystal as quantified with quasi-static nanoindentation and atomic force microscopy. Dynamic deformation in PBX materials was studied using the IMPact system for ULtrafast Synchrotron Experiments (IMPULSE) at the Advanced Photon Source. IMPULSE consists of a light gas gun which fires a projectile at a stationary target while imaging the impact event using ultrafast imaging (153 ns frame rate). Shock events such as dynamic cracking, massive plastic deformation, spallation, and impact were clearly observed in PBX and other materials even at these ultrafast time scales. These characterization techniques show the ability to establish relationships between formulation processing, mesoscale structure, and mechanical properties from static to ultrafast regimes.

XCP**Computational Physics Division**

LA-UR 13-24848

Name: **Brandon Chabaud**
Groups: **XCP-1 and T-3**
Mentors: **Jerry Brock and Todd Williams**
Field of Study: **Mathematics and Computer Science**
Discipline: **Mathematics**
Appointment: **Postdoc Research Associate**
Abstract Title: **Verifying LANL Physics Codes: Benchmark Analytic Solution to the Dynamic Sphere Problem**

Abstract

Developing benchmark analytic solutions for problems in solid and fluid mechanics is very important for the purpose of testing and verifying computational physics codes. In order to test the numerical results of physics codes being developed at LANL, we consider the small-deformation dynamic sphere problem. We present an exact solution to this problem for a visco-plastic material exhibiting isotropic symmetry. The sphere is subjected to displacement, strain, or stress boundary conditions and is governed by the momentum equation of linear solid mechanics and two constitutive equations for the plastic strain. The solution takes the form of an infinite series of eigenfunctions. The time-dependent coefficients of the eigenfunctions are governed by a second-order ODE. After demonstrating convergence under eigenmode, spatial, and time refinement, we compare the solution to numerical results obtained from the FLAG physics code.

XCP Computational Physics Division

LA-UR 13-22432

Name: **Jessica Baumgaertel**
Group: **XCP-6**
Mentor: **Paul Bradley**
Field of Study: **Physics**
Discipline: **Plasma Physics**
Appointment: **Postdoc Research Associate**
Abstract Title: **Evaluating the MMI Diagnostic on OMEGA Direct-Drive Shots**

Abstract

The Defect-Induced Mix Experiment (DIME) project conducted several symmetric direct-drive shots on the OMEGA laser in order to test a new diagnostic, the Multiple Monochromatic Imager (MMI). The MMI provides both spatially and spectrally resolved data of the capsule implosion and the resultant dopant emissions. Capsules had radii of about 430 microns, which were CH shells with an inner layer doped with 1-2 atom% Ti, and a gas fill of 5 atmospheres deuterium. Here, simulations of the target implosion by the radiation-hydrodynamics code HYDRA are post-processed with an MMI synthetic diagnostic tool and quantitatively compared to the MMI data.